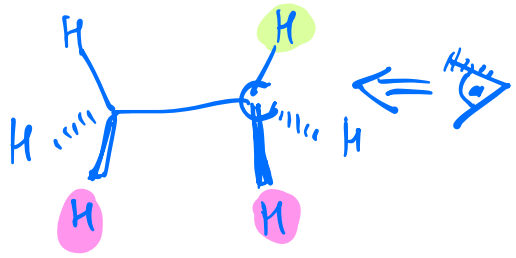
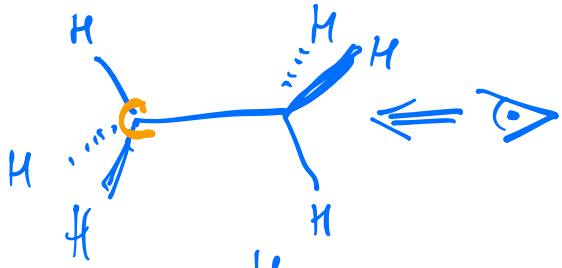
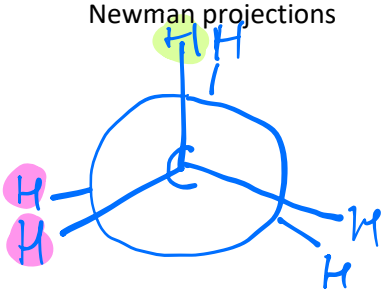
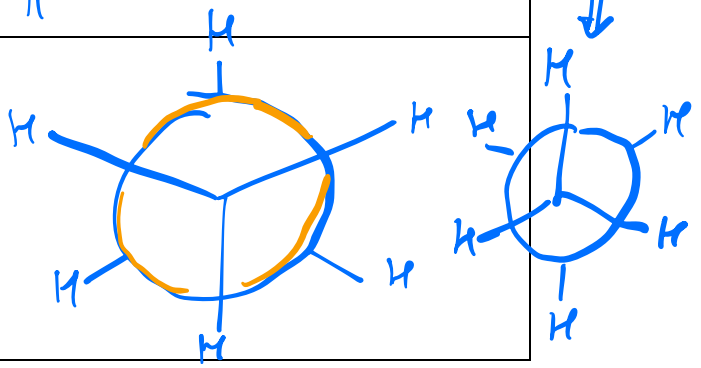
Alkane and Cycloalkane Conformations

A. Alkane Conformations

1. Bond rotation

a) Ethane

-two basic conformations relative to the alignment of protons

eclipsed	staggered
	
Newman projections 	

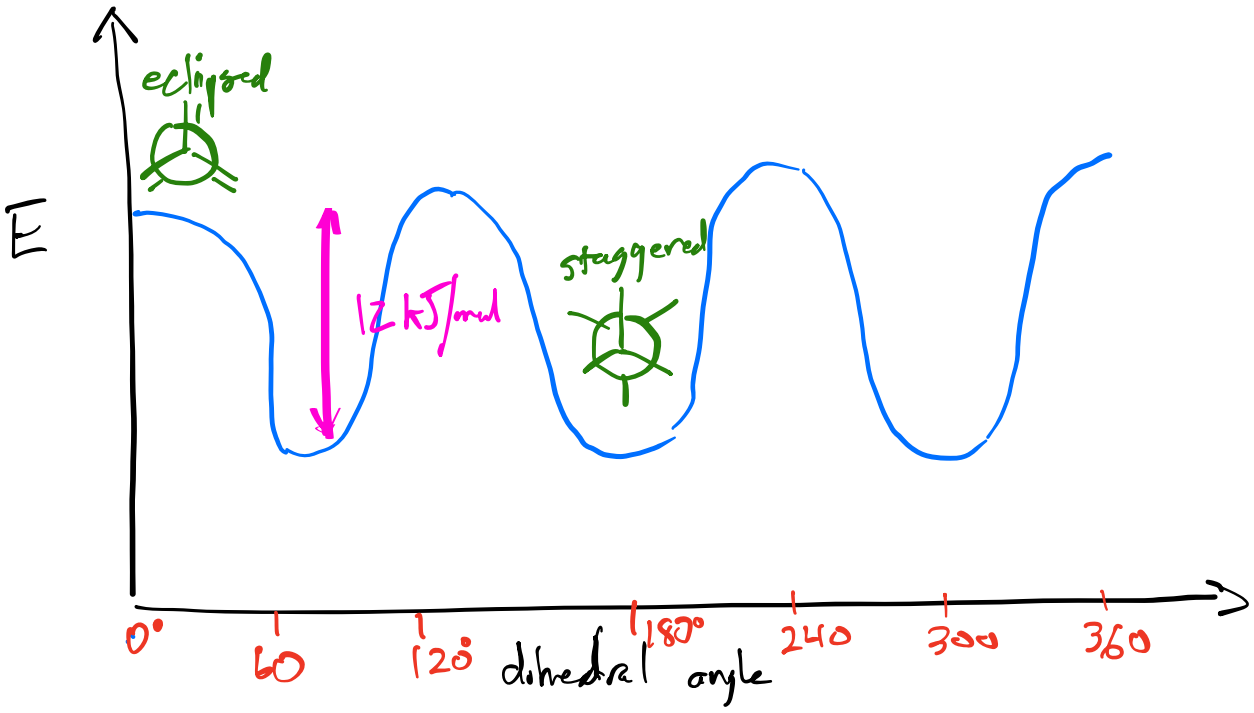
also staggered

-staggered is preferred by ~12 kJ/mol (~3 kcal/mol)

-higher E associated with eclipsed conformation is called torsional strain.

[E available at room temp. is ~80 kJ/mol or 20 kcal/mol]

Conformational analysis energy diagram for ethane

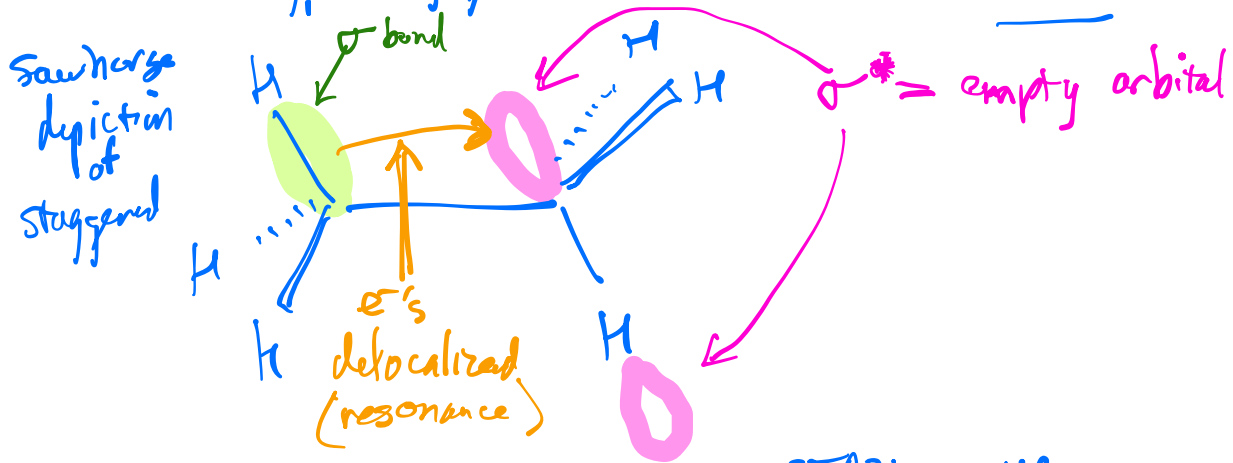


b) Basis of preference for staggered
-What do you think drives this preference?

Two reasons advanced:

(1) Preference is due to avoidance of e⁻/e⁻ repulsion.

(2) hyperconjugation between C-H sigma bond and C-H sigma* on adjacent C:

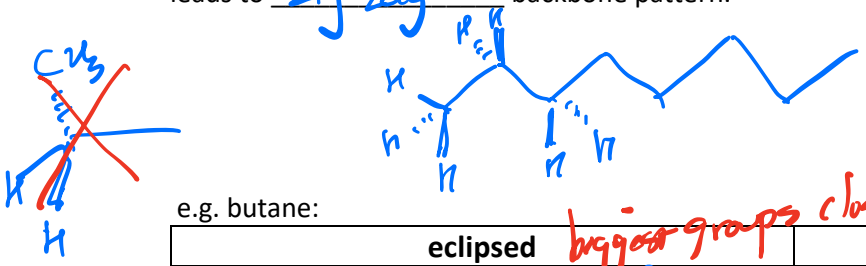


Key concept: Delocalizing or sharing electrons is STABILIZING!!!

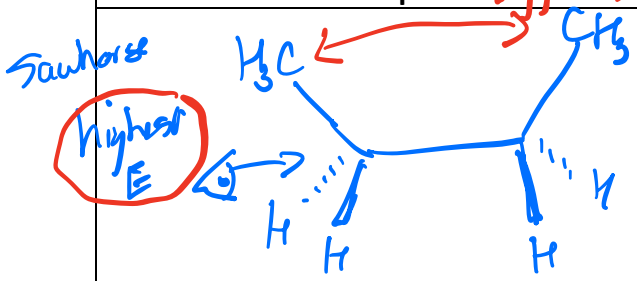
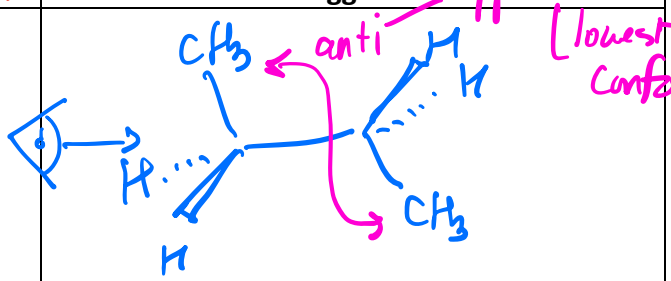
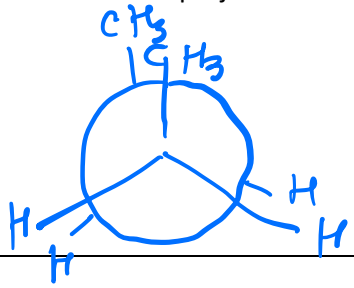
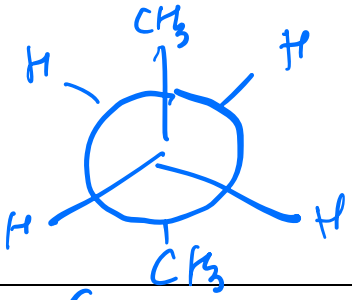
(sharing is caring!)

c) Larger alkanes

-basically the same principle applies and alkanes prefer a staggered conformation. This leads to zig-zag backbone pattern.

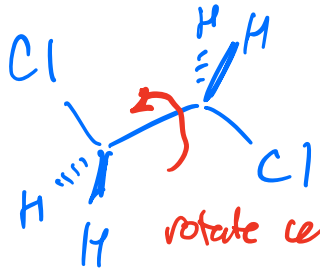


e.g. butane:

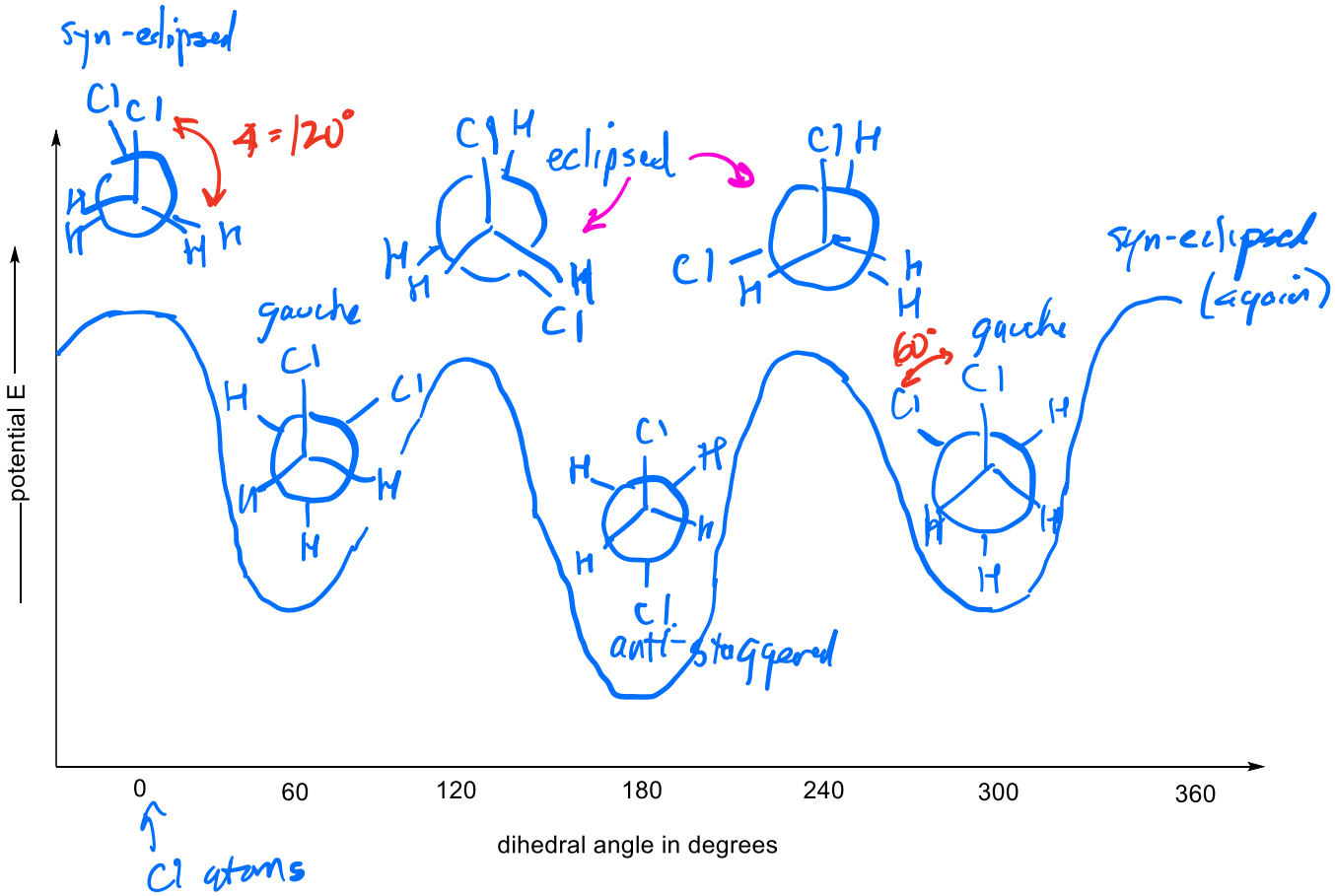
eclipsed	staggered
	
Newman projections	
	

-one little additional orientation: anti vs. gauche conformations

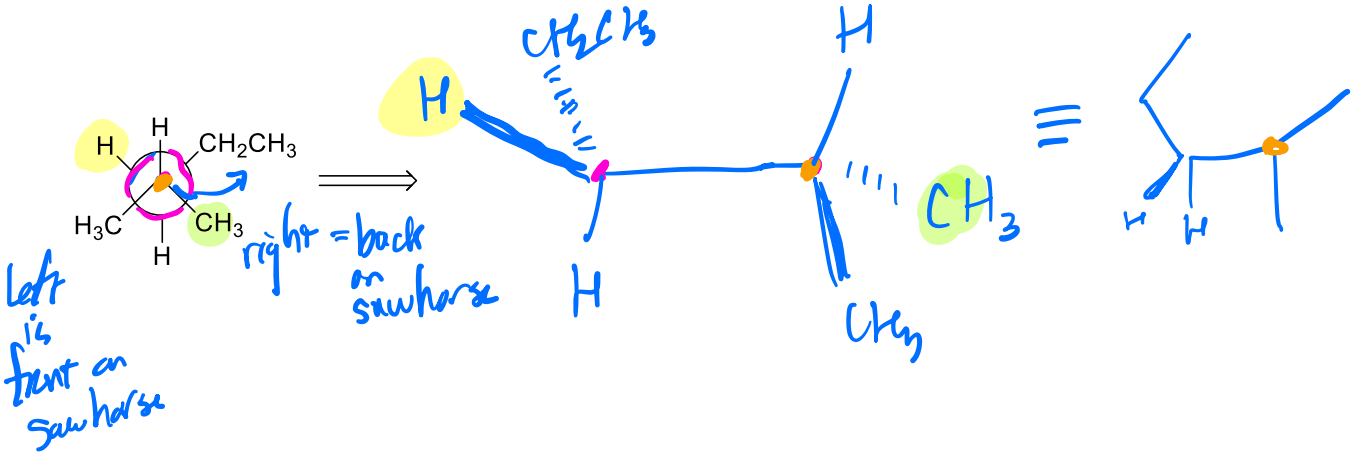
-Conformational energy diagram for 1,2-dichloroethane conformers:



rotate center σ_{C-C} bond to get different conformers



Newman projections→Sawhorse depiction



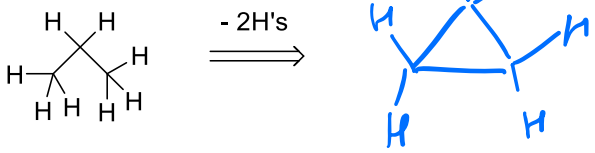
B. Cycloalkanes and Their Conformations

relative to cyclohexane

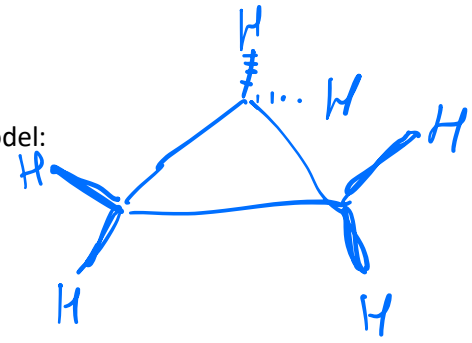
Ring	Ring size	ΔH_f per $-CH_2-$ (kJ/mol)	Ring strain energy per CH_2 (kJ/mol)
cyclopropane	3	18	38
cyclobutane	4	7	28
cyclopentane	5	-16	5
cyclohexane	6	-21	0
cycloheptane	7	-17	4
cyclooctane	8	-16	5

1. Cyclopropane, the simplest cycloalkane

a) Introduction



Draw pseudo-3 D model:



b) Ring Strain

(1) Angle strain:

-What will the C-C-C internal angles of cyclopropane? 60°

-What is the hybridization of the C atom? sp^3

-What angle does that hybridization of C prefer? 109.5°

*This difference.... in actual C-C-C angle vs. the desired sp^3 angle leads to angle strain.

(2) torsional or steric strain

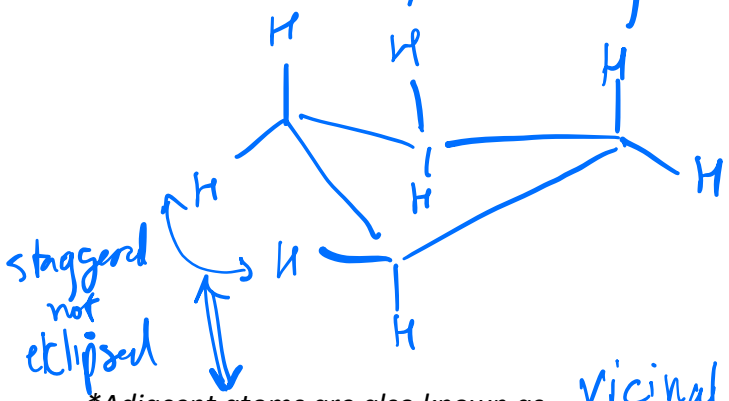
-What do you notice about the H atoms? eclipsed, not staggered → torsional strain

2. Cyclobutane and Ring Strain

a) Ring strain....

(1) angle strain? a little... 90° vs. 109.5° for sp^3 C

(2) torsional strain? Yes, but the ring reduces torsional strain by puckering



convention: no dashes + wedges

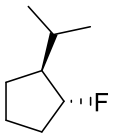
*Adjacent atoms are also known as vicinal.

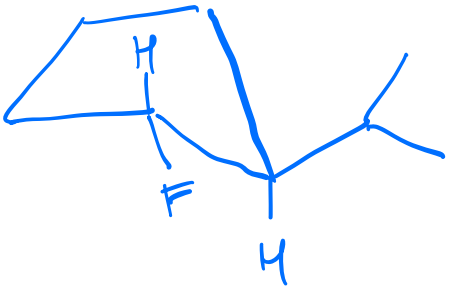
3. Cyclopentane

a) Ring Strain
-angles? 108° preferred? 109.5° → not bad

-torsional strain? Some, but ring puckers or takes an envelope shape to limit some eclipsing

a)





b) Conformations

- ring puckers to remove some eclipsing interactions + pucker often moves around ring

4. Cyclohexane

a) Ring Strain

- no angle strain → in chair structure bond angles are 109.5°!
- no torsion strain

b) Drawing Cyclohexane (Find your inner artist!)

-note equatorial and axial groups!

Reason for names:

c) Conformations of Cyclohexane

-show: chair form, twist boat, boat

-interconversion and energy relationship → Called the _____

Important notes:
1)

2)

*boat structure also has _____ interactions on sides!

Youtube video with cyclohexane chair flip:
http://www.youtube.com/watch?v=38YKPG1r30Q
or http://www.youtube.com/watch?v=DuX32urvZvQ

Expectations: Know how to draw chair and boat structures.

5. Monosubstituted Cyclohexane

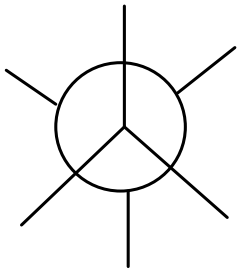
-preference for equatorial position to reduce _____

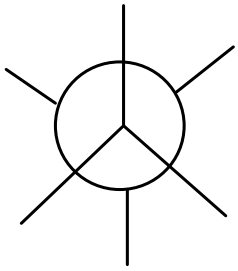
a) 2 reasons for equatorial preference

(1)

(2)

-show example:



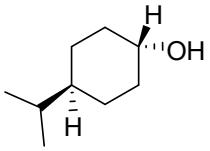


6. Disubstituted Cyclohexane

-preference for two groups to be equatorial or largest group to be equatorial

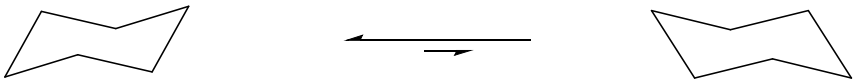
-cis vs. trans configurations:

a)



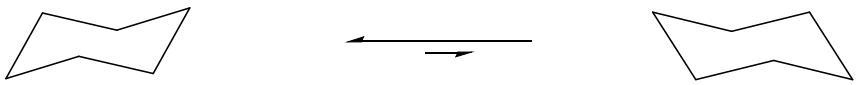
*called _____

Analyze chair structures….



Alternative depiction: Haworth projections….

b) cis isomer



7. Polysubstituted Cyclohexane

-same principles apply
-example: D-glucose

Special case: tert-butyl group ➔